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Turning Down the Volume on Granular Materials

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When confronted with a system of many discrete, interacting objects, physicists instinctively reach for ideas from statistical mechanics. Our response to granular materials, such as sand, sugar, flour, has not been an exception. But these materials possess certain characteristics, such as being inherently dissipative, that render inapplicable many key concepts, such as thermal equilibrium, the equivalence of time and ensemble averages, etc. To use statistical mechanics, therefore, certain fundamental concepts need to be modified or redefined. But no one knows how to do this in a way that yields a theory that is clear, general, and powerful. There are, however, many proposals. One of the most influential was first presented in 1989 by Sam Edwards and co-workers [1,2] at Cambridge, who proposed a statistical mechanics of powders where the volume takes the role of the energy in the usual statistical mechanics. Recently, Raphael Blumenfeld and co-workers, a colleague of Sam Edwards, also at Cambridge university (and other places), has proposed to reformulate Edward's proposal by replacing the volume with another function related to the structure of the powder. [3] It is too early to tell where this new proposal will lead, but it does have certain promising characteristics.

Edwards' original proposal is confined to stationary powders. He proposed to put the volume V of the powder in analogy with the energy U of a statistical mechanical system. Just as the macroscopic energy is the sum of the energies contained in the microscopic degrees of freedom, so the total volume of the powder is the sum of the volumes occupied by of grain-scale, "structural" degrees of freedom. In both cases, for each macrostate (specified by total energy or volume), there correspond many microstates (specified by the energy or volume of each microscopic degree of freedom). One can therefore define an entropy $S(V)$ that is the logarithm of the number of microstates with the same total volume V . This is the point of entry into the formalism of statistical mechanics: it is then possible to define a temperature-like quantity, the compactivity $X = \partial S / \partial V$, that controls the probability that a given micro-state will be realized through a Boltzmann-like factor $e^{-V/\lambda X}$, with λ a constant.

It would be quite alarming if this theory were to work in a precise and detailed way because it involves several extraordinary hypotheses. For example, implicit in the role of the compactivity as a

control variable, is the “canonical hypothesis”, namely that Boltzmann factor governs the probability that a given microstate be realized. In the usual statistical mechanics, the Boltzmann factor appears when a small “system of interest” exchanges energy with an enormous “heat bath” that imposes its temperature on the system. Thus the energy of the system fluctuates even though the total energy of the universe (system plus bath) is strictly constant, and the probability of the system states is proportional to the Boltzmann factor even though all allowed states of the universe are all equally probable. Even though our eyes are fixed on “the system”, the resulting canonical ensemble is all about “the bath”. Now, in the case of the proposed volume statistical mechanics, interaction with a “volume bath” is replaced by stirring, pouring or shaking the powder. It would be quite remarkable if these operations were equivalent to placing the powder in contact with an enormous sand pile with which it exchanges volume! Fortunately, the canonical hypothesis seems to be false. [4]

Nevertheless, the theory has been successful in that it has raised many questions and suggested new ways of interpreting data. In addition to provoking tests of its assumptions [4], experimentalists have developed for ways to measure compactivity [5], and the distribution of volume occupied by particles has been scrutinized [6].

The theory also raises the question of the elementary degrees of freedom needed to specify a granular structure. These would be the analogies of the velocity components in an ideal gas. The usual approach is to use a Voronoi tessellation to attribute the space empty space to the nearest grain. Then the grain volumes (the grain plus its neighboring empty space) are considered as a elementary volumes. The total volume of the packing is thus summed in the same way that it is constructed: grain by grain.

For many years, Blumenfeld and co-workers have been pursuing an alternative approach based on vectors connecting the intra-granular contacts. [7,8] These vectors can also be used to partition the volume, and also encode structural information about the packing, such as the average number of contacts. But as the authors point out in their recent paper [3], considering these vectors as fundamental degrees of freedom for calculating the volume leads to a strange paradox: the volume does not depend on most of these vectors. Indeed, it depends only on those at the surface of the pile, since those in the interior can be modified arbitrarily without affecting the total volume. The authors conclude that the volume is therefore not a suitable quantity for granular statistical mechanics. Instead we should consider the sum of the squares of these vectors.

Mathematically, this new quantity, called the “connectivity function” does indeed resemble many forms of energy, as it is a sum of squares. This probably gives it many convenient properties, facilitating analogies with other branches of physics. Furthermore, its connection to the contacts means it encodes information about how the packing supports loads, and could be related to the stored elastic

energy or the stress tensor, which can be written as sums over contacts. It could thus enlarge the scope of granular statistical mechanics, (hitherto confined to perfectly static piles) to address the important questions of loading and destabilization of granular materials.

On the other hand, the connectivity has no obvious macroscopic meaning, as the volume did. And this highlights a problem with the program of “granular statistical mechanics”, namely that there is no “granular thermodynamics.” Before they were statistical mechanical quantities, the internal energy, entropy, and temperature were macroscopic ones that control the interactions between many very diverse systems (even black holes have a temperature). The analogous quantities in “granular statistical mechanics” are not so powerful. It is very difficult to imagine how two piles of grains would equilibrate by exchanging volume or connectivity for example. It is clear that a satisfying statistical mechanical description of granular materials has yet to be found, and new ideas are needed.

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